Lab Receives Three-year Funding for Computing Research

Ames Lab will be able to scale up its efforts to develop advanced scientific computing codes that can take advantage of today's extraordinary progress in computing technology thanks to the Department of Energy's Scientific Discovery through Advanced Computing initiative. SciDAC awards totaling $57 million have been given to 13 DOE laboratories and more than 50 colleges and universities to support research designed to improve software for high-performance computing systems — terascale computers capable of doing trillions of calculations per second.

The development and enhancement of scientific simulation codes is a major thrust of the SciDAC program. Increasing the efficiency of codes used to model physical, chemical and biological systems is essential to scientists' efforts to address ever larger and more complex problems, such as gaining better insights into the energy-related processes of combustion, catalysis and photochemical energy conversion.

The Lab will receive about $1.35 million in SciDAC funding from the DOE over a three-year period. The funds will be used for two projects to help achieve SciDAC goals. In one project, scientists will work to develop highly scalable computational chemistry simulation codes capable of predicting energy surfaces of very high accuracy in both ground and excited electronic states. (Scalable refers to the ability to increase, or 'scale up,' computer processing power to run the same job in less time.) "Such advances in computational chemistry would tie together with advances in scalable computing — they really feed off of each other, so our project will include a lot of interaction with the Lab's Scalable Computing Lab," says Mark Gordon, program director

of Applied Mathematics and Computational Sciences. Gordon is a principal investigator on the computational chemistry project, which includes co-principal investigators Klaus Ruedenberg and James Evans and associate scientist Mike Schmidt. "We're all interested in developing extremely high levels of theory into scalable code that will allow scientists to do very accurate calculations on much larger chemical systems," Gordon continues. "That means we'll be able to attack more complicated problems."

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–Brett Bode

The Lab's second SciDAC-funded project will address the software needed to effectively manage and use terascale computational resources. The project will also include six other DOE labs and the National Center for Supercomputing Applications. Although all of these facilities are involved in building and managing large-scale parallel systems, none of them has the tools to manage those systems effectively, says associate scientist Brett Bode. "Many of the servers that are currently operating were not designed with the scalability that is needed today," notes Bode. "They can handle requests from a dozen or two computer nodes without any problem. But when you start throwing hundreds of nodes at the same software on the same server, it really no longer has the ability to cope. The programs just weren't designed to accommodate that number of requests that fast, which can lead to slowdowns and major problems."

Bode is one of the principal investigators heading up the extensive collaborative effort that will address this situation by creating a virtual Scalable Systems Software Integrated Software Infrastructure Center. The ISIC will develop an integrated suite of scalable system software components to ease the management of high-end computing systems with thousands of processors. Many of these systems are located at government agencies with large-scale computer centers like those of the DOE.

"The Scalable Systems Software ISIC is really aimed at the core of what SciDAC was intended to be, and that is a focused effort on improving software on high-performance computing systems," says Bode. "By the time we're done with the full software package, we will be able to deliver computing cycles on high-performance parallel systems to application users on these systems much more effectively. And we believe this will enable the next generation of parallel computing systems." ■

~ Saren Johnston

Brett Bode (left) and Mark Gordon